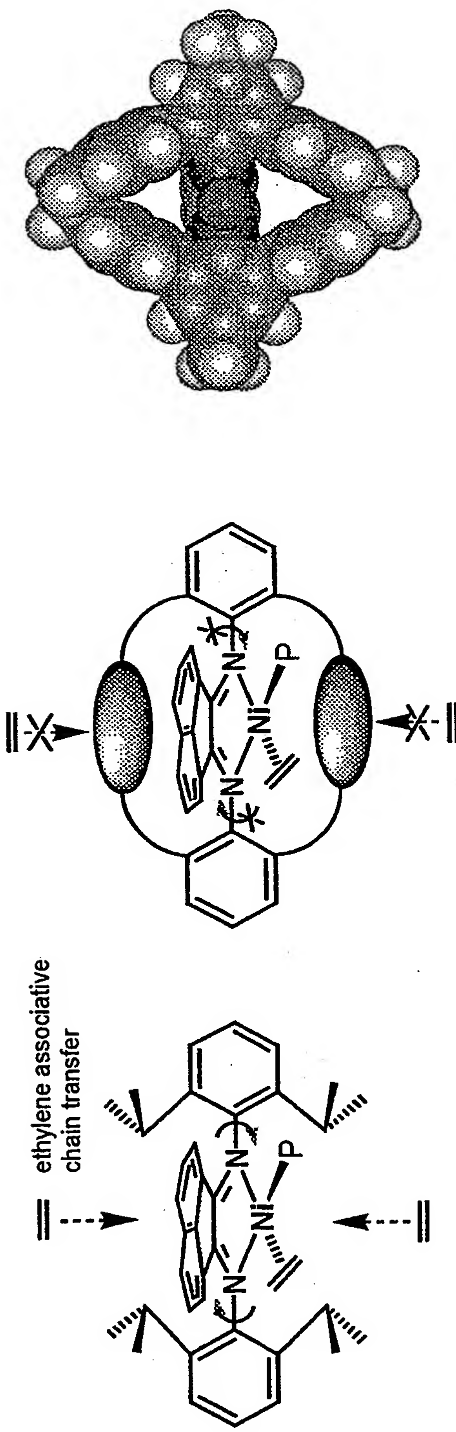
FIG. 1



A. Acyclic α-diimine complex (catalyst **4g** in reference 5)

B. Cyclophane-based α-diimine complex

C. Molecular model of complex 1

FIG. 2

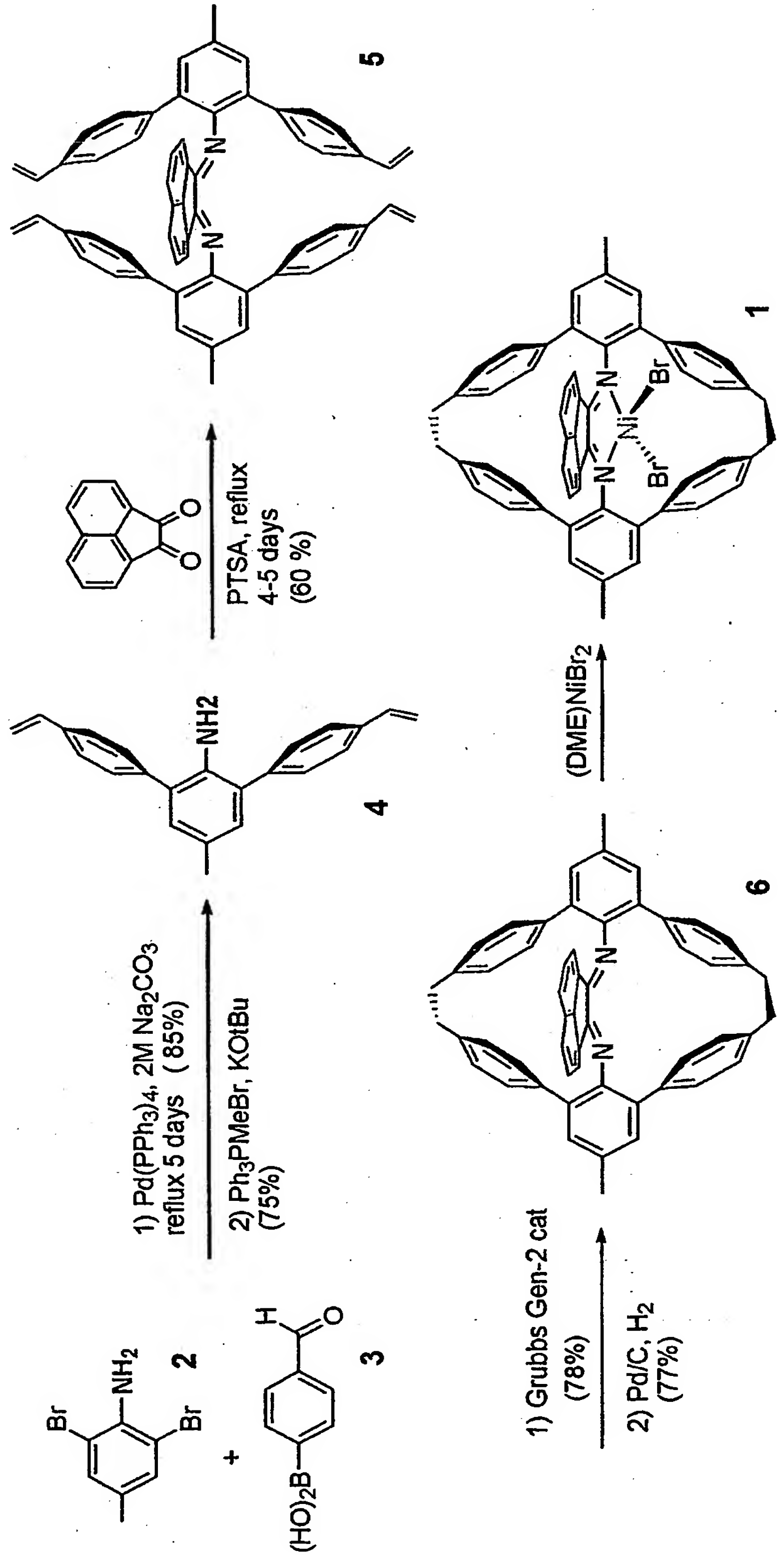

Br
NH_2
Br
2
+
$(HO)_2B$
H
O
3
1) $Pd(PPh_3)_4$, 2M Na_2CO_3
reflux 5 days (85%)
2) Ph_3PMeBr, KOtBu
(75%)
NH2
4
PTSA, reflux
4-5 days
(60 %)
N
N
5
1) Grubbs Gen-2 cat
(78%)
2) Pd/C, H_2
(77%)
6
$(DME)NiBr_2$
Ni
Br
Br
1

FIG. 3

Summary of Polymerization Data

Entry	Moles of Catalyst ($\times 10^{6}$)	Temp. (°C)	Time (min)	Yield (g)	TON[b] ($\times 10^{-3}$)	TOF[b] ($\times 10^{-3}$/h)	M_n ($\times 10^{-3}$)	M_w ($\times 10^{-3}$)	PDI	Branches Per 1000 carbons
1	1	30	5	3.48	124	1 491	320	413	1.29	66
2	1	30	10	6.70	239	1 436	288	374	1.30	73
3	1	30	15	9.25	331	1 321	294	386	1.31	67
4	1	50	5	3.20	114	1 371	248	305	1.23	80
5	1	50	10	6.85	245	1 468	652	834	1.28	84
6	1	50	15	9.00	321	1 286	342	422	1.23	85
7	1	70	5	3.11	111	1 333	323	468	1.45	91
8	1	70	10	6.10	218	1 307	619	886	1.43	89
9	1	70	15	7.35	263	1 050	429	605	1.41	91
10	1	90	5	2.50	89	1 071	252	433	1.72	97
11	1	90	10	4.70	168	1 007	462	756	1.64	96

[a] Experimental condition: in 200 mL of toluene, cocatalyst MMAO (Al:Ni ≈ 3000), 200 psi ethylene pressure.

[b] TON = turnover number, which was calculated as the moles of ethylene per mole of catalyst; TOF = turnover frequency, i.e., TON per hour.

FIG. 4A

Examples of bidentate ligands

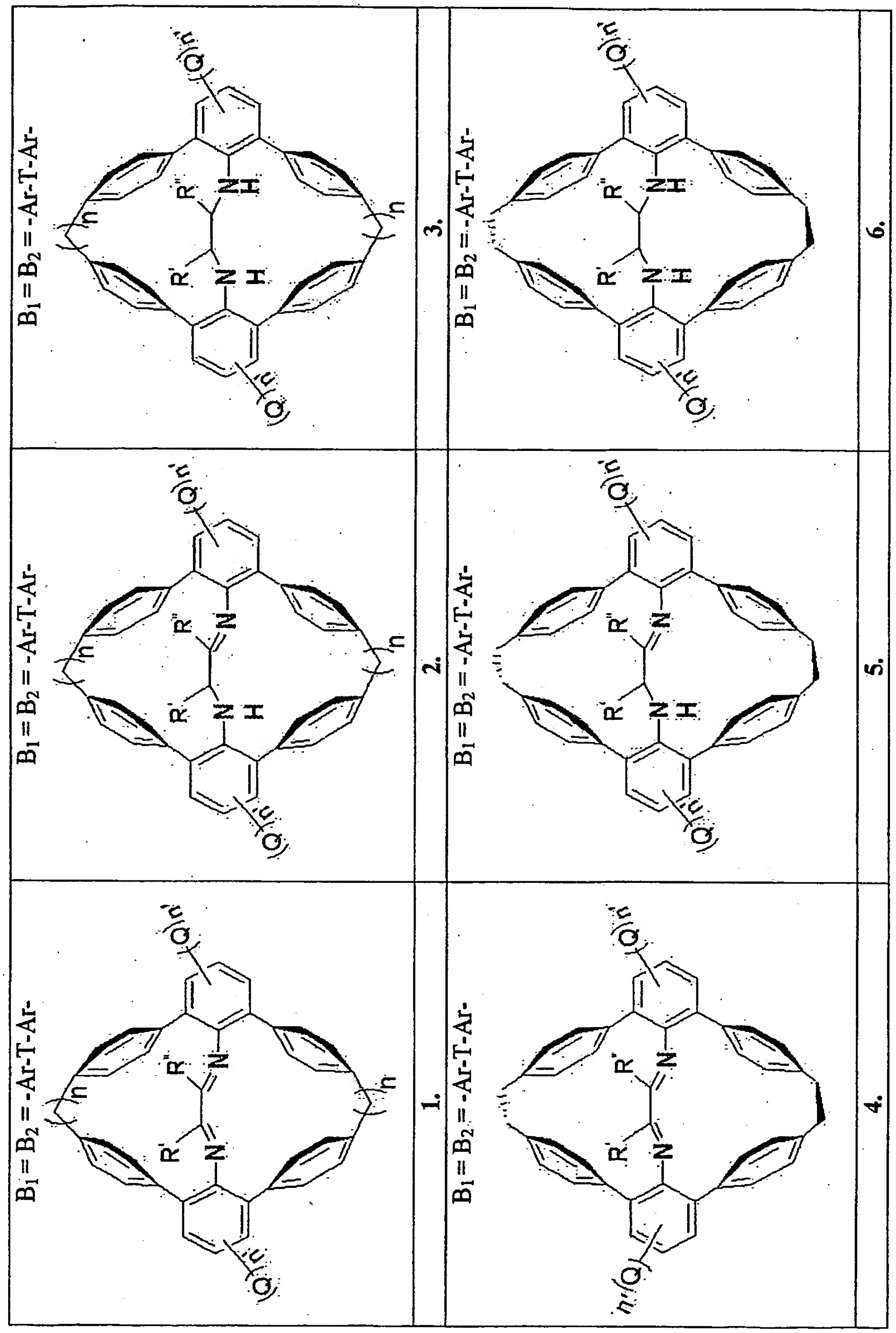
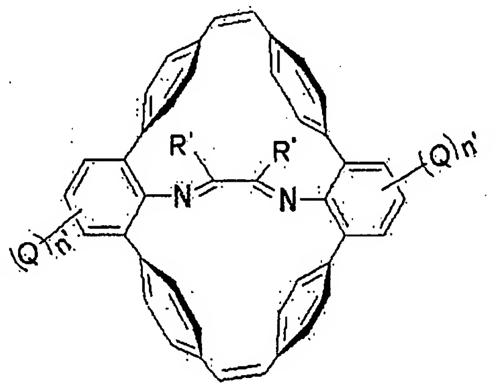
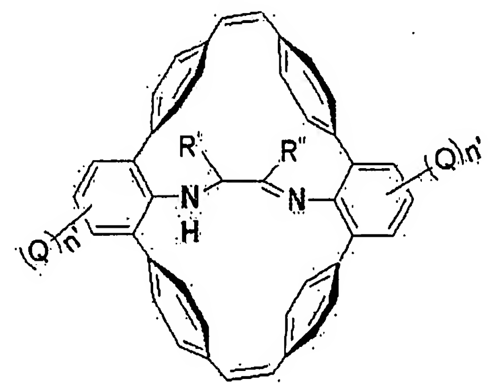


FIG. 4B

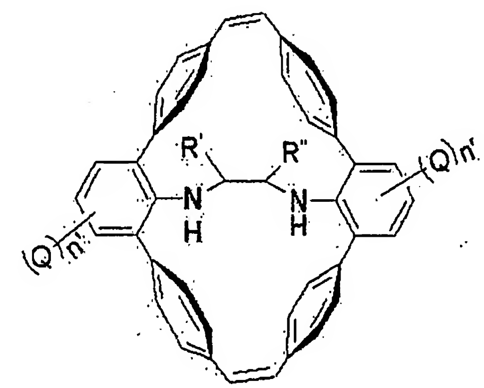
Examples of bidentate ligands (continued)



7.

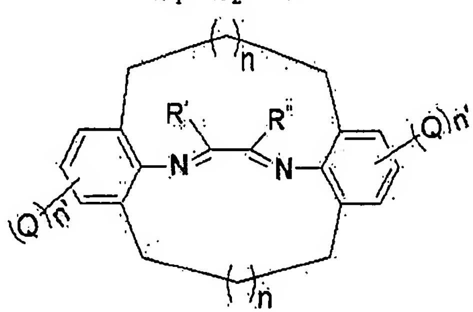


8.



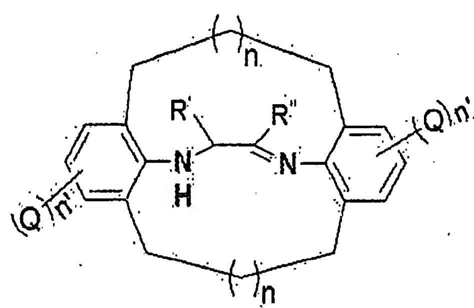
9.

$B_1 = B_2 = -T-$



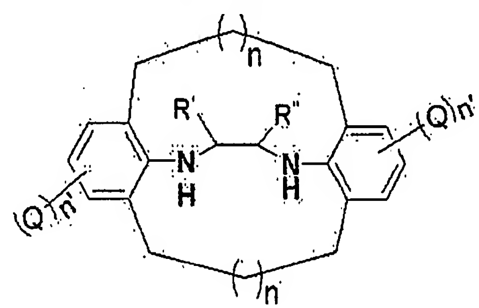
10.

$B_1 = B_2 = -T-$



11.

$B_1 = B_2 = -T-$

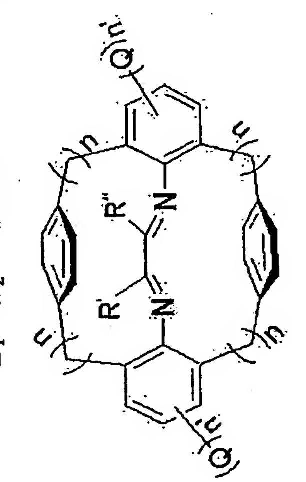


12.

FIG. 4C

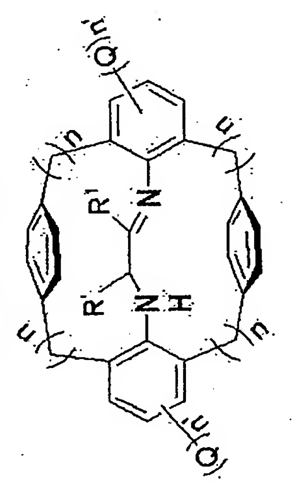
Examples of bidentate ligands (continued)

$B_1 = B_2 =$ -T-Ar-T-



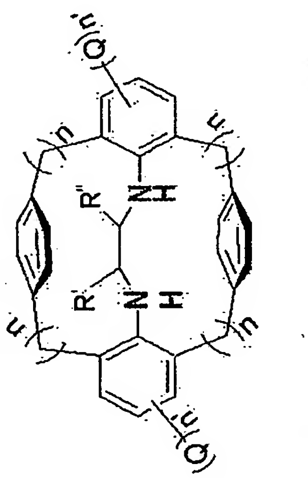
13.

$B_1 = B_2 =$ -T-Ar-T-



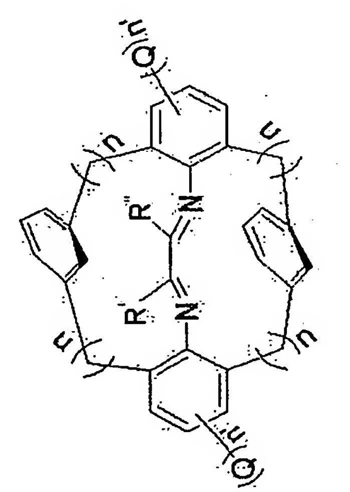
14.

$B_1 = B_2 =$ -T-Ar-T-



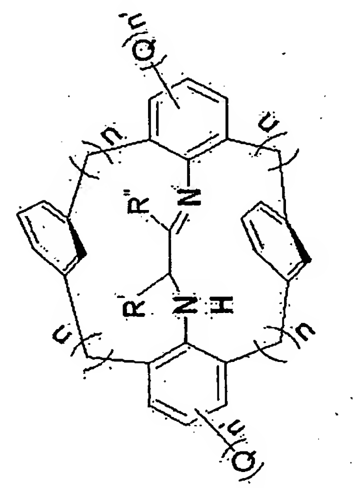
15.

$B_1 = B_2 =$ -T-Ar-T-



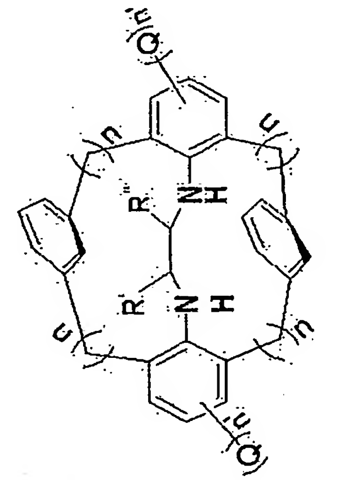
16.

$B_1 = B_2 =$ -T-Ar-T-



17.

$B_1 = B_2 =$ -T-Ar-T-



18.

FIG. 4D

Examples of bidentate ligands (continued)

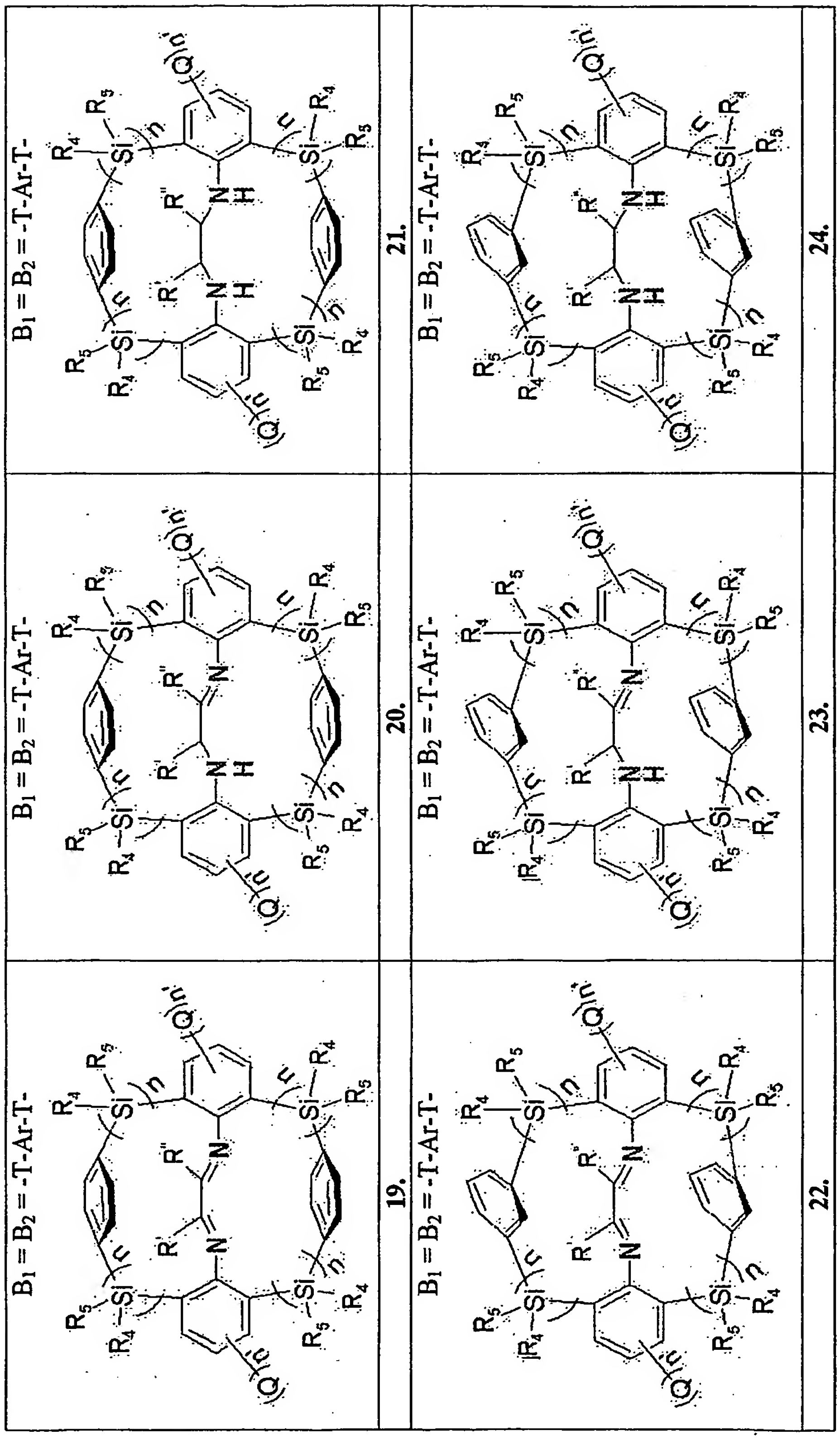
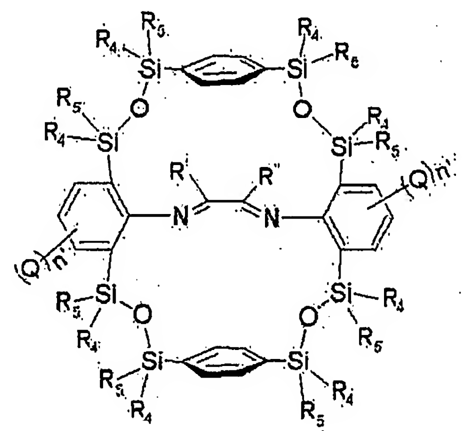


FIG. 4E

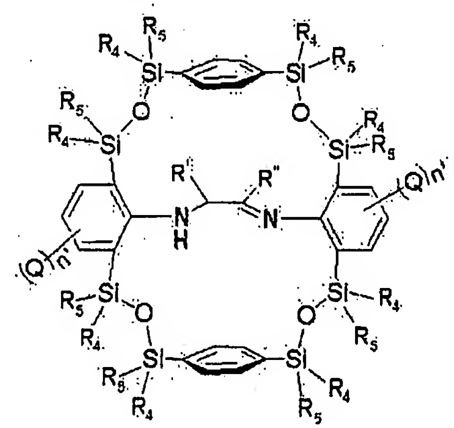
Examples of bidentate ligands (continued)

$B_1 = B_2 = $ -T-Ar-T-



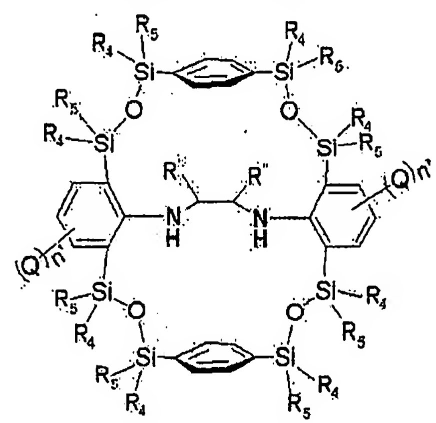
25.

$B_1 = B_2 = $ -T-Ar-T-

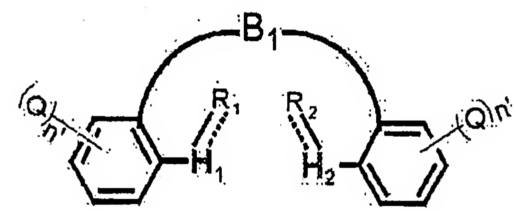


26.

$B_1 = B_2 = $ -T-Ar-T-



27.

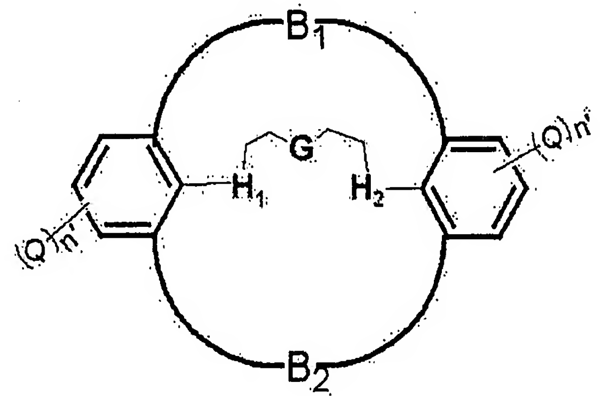


half-cyclic structure for any of the above ligands

28.

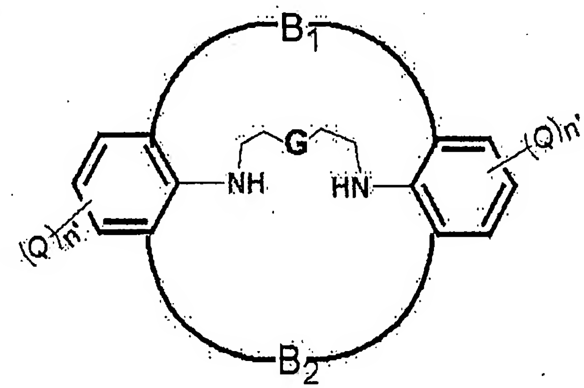
FIG. 5A

Examples of tridentate ligands



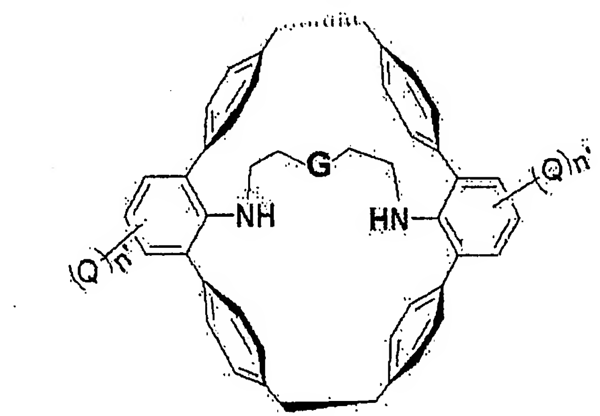
H_1, H_2, G = Heteroatoms selected from O, P, S, N, etc.

29.



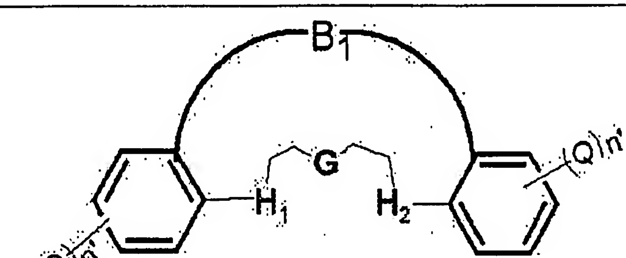
G = Heteroatoms selected from O, P, S, N, etc.

30.



G = Heteroatoms selected from O, P, S, N, etc.

31.

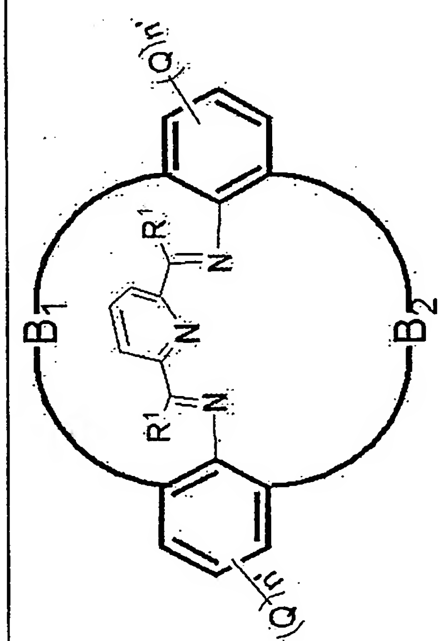


H_1, H_2, G = Heteroatoms selected from O, P, S, N, etc.

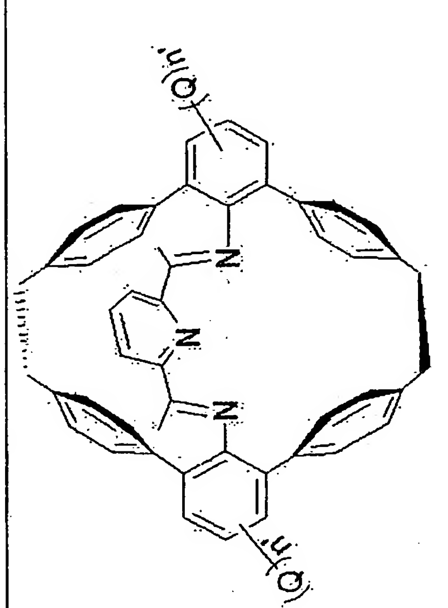
32.

FIG. 5B

Examples of tridentate ligands (continued)



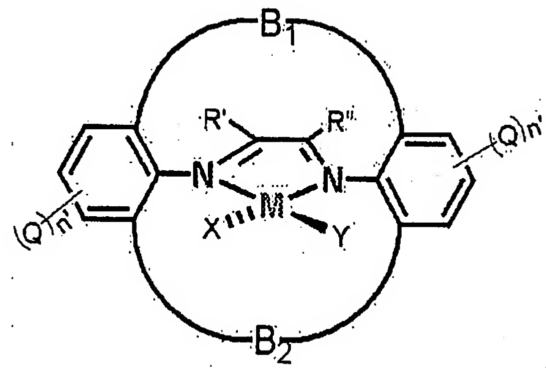
33.



34.

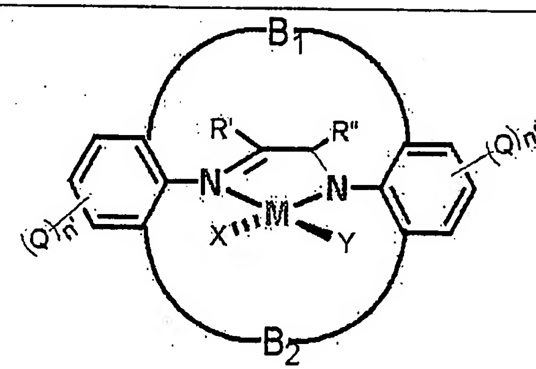
FIG. 6A

Examples of preference of metals for different types of ligands



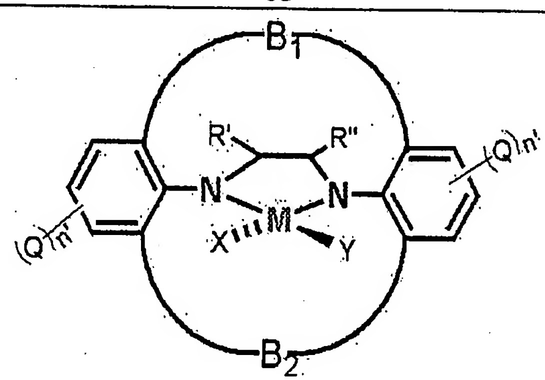
For this type of ligand, preferred M are late transition metals such as Fe, Ru, Os, Rh, Ir, Ni, Pd, Pt, Cu, and most preferred are Ni and Pd.

35



For this type of ligand, preferred M are Zn and Al.

36



For this type of ligand, preferred M are early transition metals such as Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, and W, and most preferred are Ti, Zr, Hf, V, and Cr.

37

FIG. 6B

Examples of preference of metals for different types of ligands (continued)

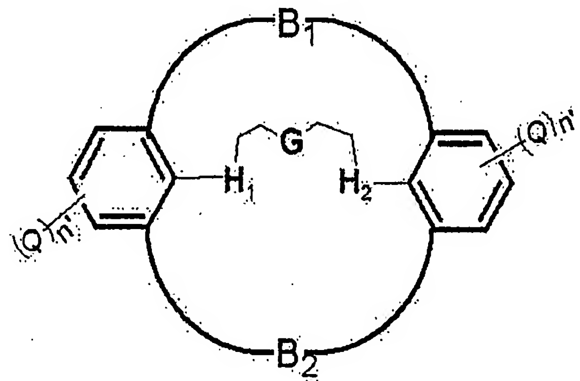
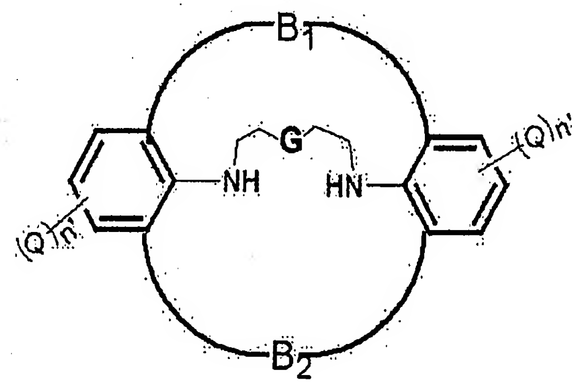
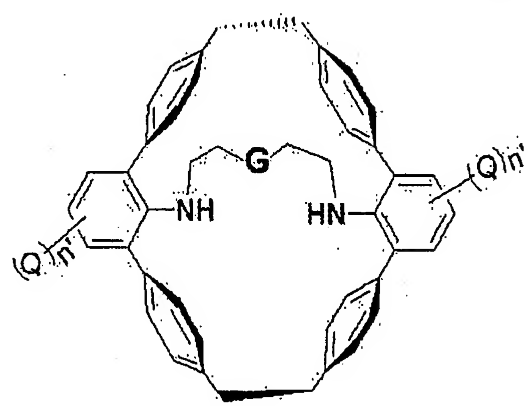
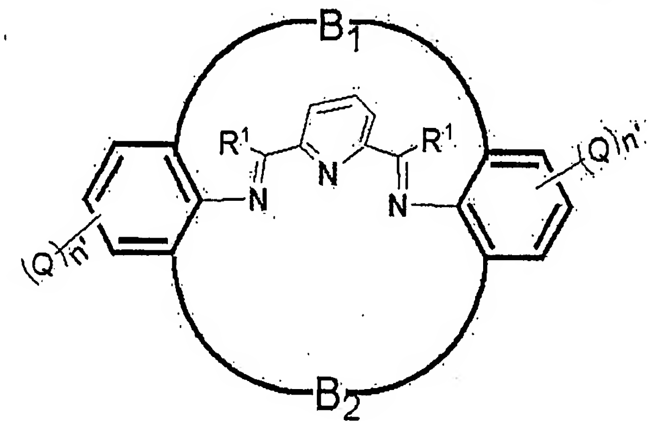
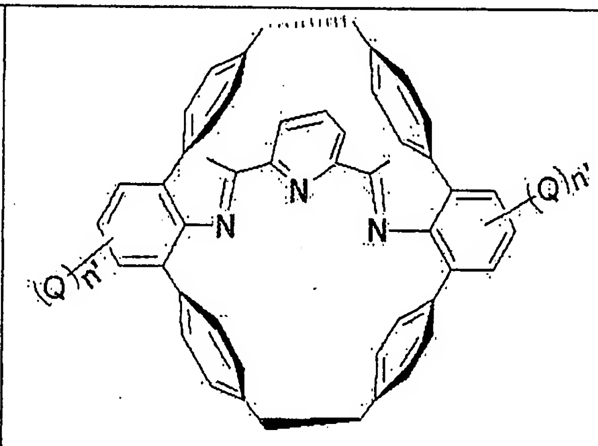
 H₁, H₂, G = Heteroatoms selected from O, P, S, N, etc.	 G = Heteroatoms selected from O, P, S, N, etc.
38.	**39.**
	For this type of ligand, preferred M are early transition metals such as Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, and W, and most preferred are Ti, Zr, Hf, V, and Cr; G = Heteroatoms selected from O, P, S, N, etc.
40.	

FIG. 6C

Examples of preference of metals for different types of ligands (continued)

	
For this type of ligand, most preferred M are Fe and Co.	
41.	**42.**

In structures 1 through 42, Q, n, R_4 and R_5 are as defined in Formula 1 in the specification, n′ is 1 through 4, and R′ and R″ are alkyl, alkenyl, aryl, aralkyl, or cycloalkyl.

FIG. 7
(Prior Art)

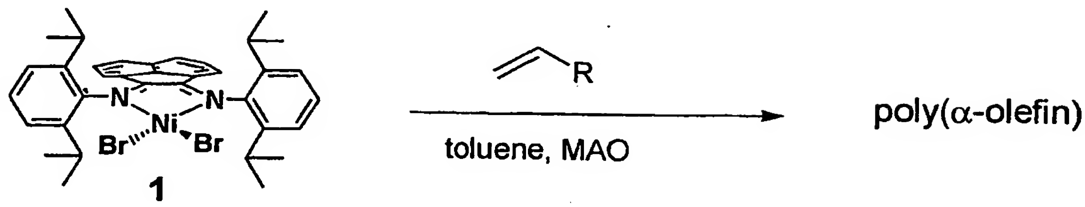


FIG. 8

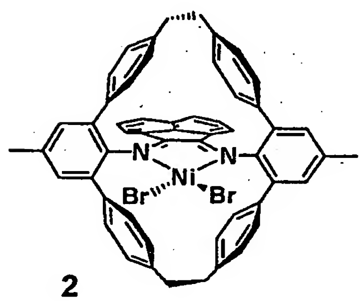


FIG. 9

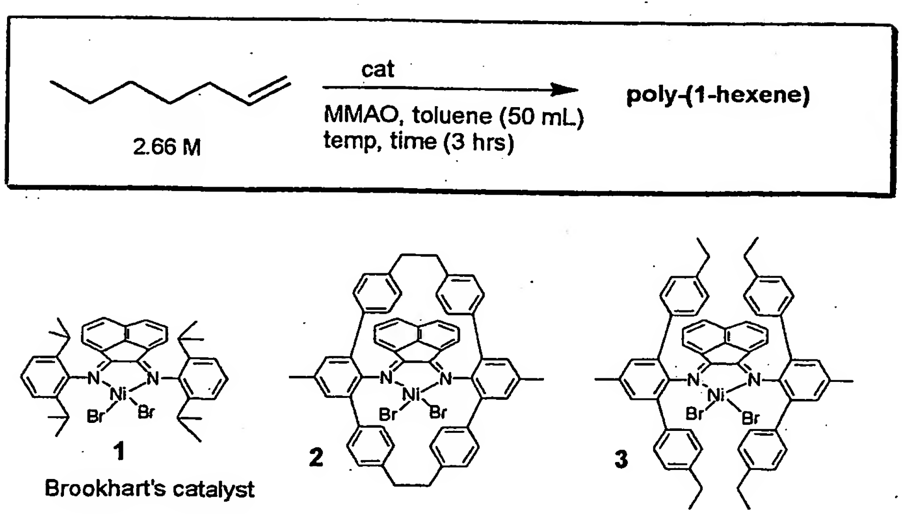
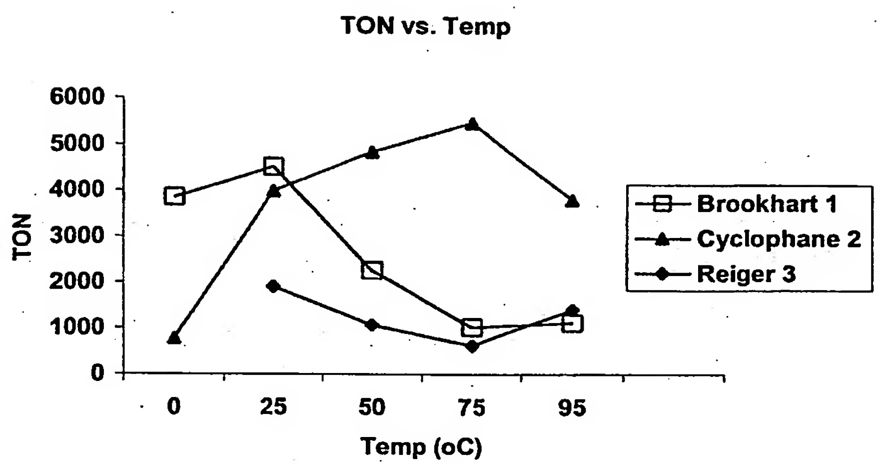


FIG. 10

Polymerization of 1-Hexene
(Catalyst Activity and Molecular Weight Data at 0 °C and at 25 °C)

entry	c at	Load (mmol)	Temp (oC)	Yield (g)	TON	Mw	Mn	PDI	DSC (°C)	Branch /1000c
F62	2	0.005	0	0.33	784	170 K	96 K	1.77	T_m 58	65
F36	2	0.01	0	0.41	488	305 K	292 K	1.05	T_m 63	61
F84	1	0.005	0	1.62	3850	719 K	627 K	1.15	T_m -42	104
Ref *JACS 95, 6414*	1	0.017 activated by Et_2AlCl	0	2.1	1468	310 K	140 K	2.2	T_m -20 T_g -57	100
F60	2	0.005	25	1.68	3992	623 K	510 K	1.22	T_m 62	57
F72	1	0.005	25	1.90	4515	817 K	543 K	1.50	T_m -50	108
Ref *JACS 96,11664*	1	0.017 3.2 M; 30 min rxn.	23	----	2800	129 K	84 K	1.54	T_m -17 T_g -57	120
F74	3	0.005	25	0.80	1901	88 K	83 K	1.06	T_m 56	35
F42	2	0.005	75	2.21	5466	622 K	529 K	1.17	T_m 59	52
F68	1	0.005	75	0.43	1022	415 K	279 K	1.49	T_m -53	111
F70	3	0.005	75	0.26	618	131 K	92 K	1.43	T_m 73	38
F46	2	0.005	95	1.6	3802	252 K	125 K	2.00	T_m 57	54
F48	1	0.005	95	0.47	1117	287 K	171 K	1.68	T_m -53	113
F50	3	0.005	95	0.59	1402	77 K	59 K	1.29	T_m 76	40

FIG. 11


TON vs. Temp
6000
5000
4000
3000
2000
1000
0
TON
0
25
50
75
95
Temp (oC)
Brookhart 1
Cyclophane 2
Reiger 3